To link to this article : DOI : 10.1016/j.cep.2008.03.016
URL : http://dx.doi.org/10.1016/j.cep.2008.03.016

Case-based reasoning and TRIZ: A coupling for innovative conception in Chemical Engineering

Guillermo Cortes Robles, Stéphane Negny*, Jean Marc Le Lann

Laboratoire de Génie Chimique (PSI – Génie Industriel), UMR-CNRS 5503, INPT-ENSIACET, 118 Route de Narbonne, Toulouse 31077, France

A B S T R A C T

With the evolutions of the surrounding world market, researchers and engineers have to propose technical innovations. Nevertheless, Chemical Engineering community demonstrates a small interest for innovation compared to other engineering fields. In this paper, an approach to accelerate inventive preliminary design for Chemical Engineering is presented.

This approach uses case-based reasoning (CBR) method to model, to capture, to store and to make available the knowledge deployed during design. CBR is a very interesting method coming from artificial intelligence, for routine design. Indeed, in CBR the main assumption is that a new problem of design can be solved with the help of past successful ones. Consequently, the problem solving process is based on past successful solutions, therefore, the design is accelerated but creativity is limited and not stimulated.

Our approach is an extension of the CBR method from routine design to inventive design. One of the main drawbacks of this method is that it is restricted in one particular domain of application. To propose inventive solution, the level of abstraction for problem resolution must be increased. For this reason CBR is coupled with the TRIZ theory (Russian acronym for Theory of Solving Inventive Problem). TRIZ is a problem solving method that increases the ability to solve creative problems thanks to its capacity to give access to the best practices in all the technical domains.

The proposed synergy between CBR and TRIZ combines the main advantages of CBR (ability to store and to reuse rapidly knowledge) and those of TRIZ (no trade-off during resolution, inventive solutions). Based on this synergy, a tool is developed and a mere example is treated.

Keywords:
TRIZ
CBR
Inventive design
Chemical process

1. Introduction

In every engineering field, researchers have to provide solutions, knowledge, evolutions, to improve the surrounding world. For companies, one way to succeed in these challenges is to innovate. Chemical Engineering does not escape to this evolution. Of course, the process industries undergo new trends imposed by the world market evolution [1]: lower profit margin, reduced time to market, decreased product life cycle, environmental constraints, sustainable development, etc. Moreover nowadays, Chemical Engineering has to face new industrial context, for example:

- Gradual falling of hydrocarbon reserves.
- Emergence of new domains of application: nano–micro technologies and biotechnologies.
- A strong need of our knowledge in some fields: energy, sustainable development.

Consequently, all these trends and demands accelerate the need for innovation and for anticipation of the future evolutions of products and processes. In the same time, these evolutions generate new design problems and increase the level of complexity of the problems to solve. Based on current knowledge, the design of unit operations or processes will have to evolve technically, technologically, and perhaps in the way to theoretically approach problems. But as Srinivasan and Kraslawski [1] underline in their introduction, the Chemical Engineering community demonstrates a weak interest in innovation and creativity comparatively to other engineering fields.

In the context described above, there is a strong need for methodologies and tools in order to propose rapidly inventive solutions for the design of any complex problems. Here two important points emerge: how can we propose rapidly a solution and reduce the time of design in one way, and how can you find an inventive solution for problems in the other way. To answer to these questions, process engineers have to manage new relevant concepts in

* Corresponding author. Tel.: +33 5 62 88 58 35; fax: +33 5 62 88 56 00.
E-mail address: stephane.negny@ensiacet.fr (S. Negny).

order to improve process industries competitiveness: innovation, creativity and technical knowledges (coming from various scientific fields). In this article, we propose a methodology (and a tool based on it) to help process engineers to accelerate complex design and to propose creative ideas. Of course, the development of this methodology must contain the main components of each support design tools, defined by Simons [2]: to propose adapted steps for design, definition of solutions, criteria to evaluate solutions.

Generally, when you face a new problem, you use your early experiences and you try to adapt them in order to produce a solution to this new problem. This analogical reasoning is the most used human being process during the problem resolution. Various methodologies and theories try to exploit this analogical reasoning for problem resolution. The main difference between them is the level of abstraction in the exploitation of knowledge. Some artificial intelligence (AI) methods, and more precisely knowledge management ones, work on knowledge inside a technical domain (Chemical Engineering for example), and more generally in a specific part of this domain (unit operations). These methods are useful for routine design. On the other hand, when you want to find non-routine solutions, you have to enlarge your field of knowledge. The TRIZ theory (detailed below) deals with this idea. TRIZ is based on the analysis of knowledge used in all technical domains. It is important to notice that the level of abstraction for problem resolution is different; inside a specific domain for AI methods and across engineering fields for TRIZ. Because of this main difference, these methodologies produce solutions with different level of innovation: incremental innovation for AI methods, and rupture one for TRIZ. After its patents analysis for the creation of TRIZ, Altshuller [3] classified the solutions according to five levels, depending on their degree of innovation (Table1).

AI methods allow to reach solutions corresponding to the first and second level and sometimes to the third one, while the TRIZ theory can generate solutions until the third level and sometimes in the fourth one for TRIZ experts. Concerning the rapidity to produce a solution, AI methods, and more specifically case-based reasoning (CBR) in this article, are more efficient than TRIZ theory.

During design process, the problem resolution phase can be decomposed in three main steps:

- Problem identification (product or process analysis).
- Problem definition and description (taking into account of constraints: environmental, economical, technical, etc.).
- Problem resolution.

During the problem resolution process, in AI methods there is a preliminary phase dealing with these 3 points: one part dedicated to the problem elaboration (identification and definition), the other part about the problem resolution. This preliminary phase is very important and can take a long time but it is only made once at the beginning, then for each new problem the description will be the same. This is due to the fact that the application of these methods is specific to one part of a technical domain. Another consequence of this technical domain specificity is that the proposed solutions are more precise and operational. Once the elaboration phase is finished, the resolution process is repeated automatically and the designer has only to fill data concerning its new problem and then to analyse, to correct and to test proposed solution.

On the rapidity point of view, the TRIZ theory has a drawback due to its level of application of knowledge. However with TRIZ, designers propose solutions more quickly than the other methods focused on creativity stimulation and innovation. With TRIZ, for each new problem faced, the whole resolution process (the main 3 steps) must be deployed, consequently it takes a lot of time. Moreover, TRIZ resolution process does not propose an operational solution but a way to explore to find an inventive solution: it places designers under good conditions by giving them some directions to let express their creativity. Consequently there is a need for an additional work to have an operational solution.

This introduction puts in highlight the need of a methodology to accelerate inventive design. Two types of methods are presented for design. The complementarities of these methods are going to be exploited in order to create this methodology. The goal of this article is to explore in more details this synergy. In this paper the advantages of CBR and TRIZ are coupled to accelerate design and to find inventive solutions in Chemical Engineering. This paper is decomposed in different parts. First (part 2), the CBR method is presented with some examples of application in Chemical Engineering. The third part deals with a detailed presentation of TRIZ, and the tools and concepts included in the synergy. The next part is dedicated to the presentation of the methodology and its implementation. Before concluding, a mere example is presented with the simulated moving bed (SMB).

2. CBR

2.1. General presentation

Artificial intelligence and more precisely knowledge management approaches try to use past experiences in a domain to solve new problems. The main difficulty is to find a way to store, retrieve and reuse knowledge accumulated in an organization. Coming from AI, CBR is one approach to manage knowledge. The main idea in CBR is that: similar problems have similar solutions. Basically in CBR, users search to solve a new problem by establishing some common characteristics between the initial problem and some previous solved ones. Then the CBR process uses and adapts earlier successful resolutions and solutions in order to solve the new problem. It imitates everyday human problem solving. CBR traces its roots to the work of Schank [4] on dynamic memory. This document [4] describes the memory-based approach to reasoning, which means that human memory is dynamic because it is continuously changing according to the new problems or situations he has to face. Consequently, these new experiences which inherently contain some lessons learned in a particular context could be used to face new ones. The CYRUS system developed by Kolodner [5] was the

Table 1
Altshuller innovation levels

Level	Description	Origin of knowledge	% of patent
1	Apparent solution: solution by methods well-known within specialty (slight changes in parameters)	A person	32
2	Small improvement: inside a paradigm: improvement of an existing system without changes in functional principle	A firm, a company	45
3	Substantial invention inside technology: essential improvement of existing system, changes in functional principle	Inside an industrial domain	18
4	Invention outside paradigm: new generation of design using science not technology	All industrial domains	4
5	Discovery: major discovery and new science (essential changes in civilization)	Set of knowledge	<1

first computer implementation of many of the schemes exposed by Schank [4]. After that, many CBR systems had been implemented in various fields. Depending on how the past experiences are reused, CBR systems can be classified in two main categories: problem solving systems and interpretative ones. The latter are limited to retrieve solutions without adaptation in order to justify or evaluate a situation. The former build a specific solution for the new problem by adaptation of previous solutions. But with our goal to propose a solution, the retrieve step alone is not enough; the solution must be modified and adapted, because the initial problem and the retrieved one do not match totally: some differences exist. Therefore we are going to implement a problem solving system.

In CBR, the central notion is a case. A case represents an earlier experience with the problem description (Pb), its associated solution (Sol) and eventually some results and comments (Co) about how the solution was obtained; like success or failure of the solution, advises of application (1). Various cases are collected and stored in a memory; the case base.

$$\text{Case(Pb, Sol, Co)} \tag{1}$$

In CBR, the new faced problem (target problem) is compared to other problems stored in the case base (source problems), and the most similar problem and its associated solution are extracted. This extracted solution (source solution) is adapted to propose a first specific solution (target solution) to the initial problem. This target solution is revised and tested, and when the target problem is totally solved, it is stored (or not) in the case base memory. Finally, this process reduces resolution time because it gives an initial guess for the target solution. And it is often more efficient to solve a problem from an existing starting point than to develop the whole solution from nothing. For a good performance of a CBR system, the case base must cover the whole or an important part of the problem space (all the problems that may appear in the specific domain of application). Consequently, the case base must contain numerous cases.

The CBR approach has been used in many fields like Cognitive Scientists, Artificial Intelligence Research, Expert Systems, and Information Technology. The approach used here, is the same developed in the artificial intelligence field. In AI, conventional approach uses knowledge model in a specific domain but it is difficult to implement because solutions must be searched in a huge space.

2.2. The CBR process cycle

The CBR method is a cyclic process, usually named 4′R, but it can be extended to the 5′R model (represented in Fig. 1), by including the preliminary step: *case representation*. This preliminary important step consists in representing the past experiences contained in cases for the reasoning purpose. Many ways for case representations are possible, but the more used is a vector of feature-value pairs for the problem and solution descriptions. The description of a case is based on the relevant features that characterised it: components, apparatus, flow rates, pressure, temperature, etc. To complete the description, the features are filled with their associated values. Consequently, the initial step before applying the CBR process is to find these relevant features for the problem and solution descriptions. Then you have to collect data to describe the target problem and to fill the target problem features with its specific values. Then the CBR cycle can start with the goal to propose a value for each feature of the target solution.

After the filling of the target problem features, the next step in the cycle consists in *retrieving* the case or a subset of cases, stored in the case base, that are relevant to solve the target problem. During the elaboration, the target problem is described by a list of features; this list is used during the retrieval step to find problems

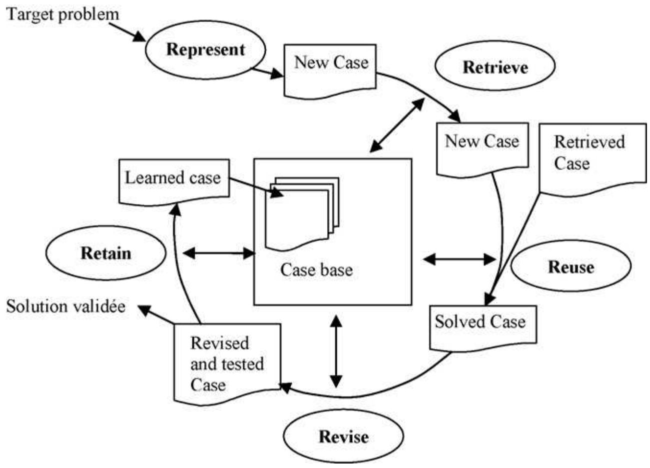

Fig. 1. The CBR process cycle.

that match with the target one. The matching is realised with a similarity function:

$$\text{SIM} = \frac{\sum_{i=1}^{n} w_i \,\text{sim}(f_i^{\text{I}}, f_i^{\text{R}})}{\sum_{i=1}^{n} w_i} \tag{2}$$

where $f_i^{\text{I}}, f_i^{\text{R}}$ represent respectively the values for the features i of the target problem (I) and the retrieved cases (R), sim is the local similarity function for this feature i and w_i is the weight of the feature i. In their article, Avramenko and Kraslawski [6] deal with the different ways to measure local similarity. It depends on the type of feature values: semantic, symbolic, numeric, etc. SIM represents the global similarity. If various similar cases are found, the global similarity function ranks them. Moreover, the global similarity function can be customised thanks to the weight, in order to give more importance to one feature to others for the research. However, during the lifetime of a CBR system, new cases can be added to the case base therefore the case base is continuously growing. Consequently, it would be time consuming to measure the similarity between the target problem and all the cases in the base. To decrease this research time, we adopt a case base indexation to filter and select the most relevant source cases and then measured the global similarity on this subset of cases. The organization of the memory is often based on the decision tree approach; the case base is successively restricted thanks to decision sequences.

The solution of the retrieved case is used as a starting point, an initial guess to the target problem. More precisely, it is used as an initialisation of the resolution because the retrieved problem does not match totally the initial one, along all the features. Consequently we need to adjust some features of the retrieved solution to answer to the target problem; *reused step*. This adaptation uses additional knowledge which can be modelised by rules, equations, heuristics, etc. Then the adapted solution is implemented, tested (by simulation, optimization, or experimental validation for examples) and repaired if necessary; it is the *revised step*. As explained above, various CBR application avoid the reused and revised steps because of the difficulty to model additional knowledge in order to do them automatically. It is particularly the case in process engineering due to the complexity of the phenomena treated.

One advantage of the CBR approach is its ability to learn with the incorporation of new cases in the case base (*retain step*). Failure like success can be stored in the memory, because we also learn from failures. With this step, the system evolves, enlarges its cover of problems and increases its performance by extending the case base. In order to avoid redundant information, saturated memory, and decreased performance during the research of similar cases, not all the cases are stored but only the most relevant ones.

2.3. Comments on CBR

CBR is widely used in different domains like medicine, food, nutrition, design, etc. More specifically, there are some applications in Chemical Engineering: equipment selection [7,8], process control [9], flowsheet design [10], process synthesis [11,12], separation design [13–15], process design [6,16], etc.

The CBR approach is very interesting for complex problem resolution because it can quickly offer a solution and accelerate design. It is based on the fact that the second time you solve a problem (or a part of a problem) you do it quicker and easier because you recall your success and your mistakes are avoided. CBR is an interesting tool to capitalize quickly and effectively knowledge. The CBR cyclic process is easy to implement, nevertheless there is two important points: the elaboration stage to identify the features to describe a case and the adaptation step to find the way to adapt the initial case; probably the most difficult part. As Lopez-Arevalo et al. [16] conclude, a designer plays a critical role during the 5′R process and its intervention is mandatory to propose one specific solution from several initial solutions.

The second main advantage of CBR is its ability to learn and consequently to manage a huge amount of information. While its specificity in a domain is an advantage, it can be a drawback too, because you do not have access to the best practices in other domains. As we explain before, the latter are important to increase the degree of inventiveness of the solution. CBR can solve problems but the proposed solutions have not a high level of innovation (in the way of TRIZ) because they are based on solved cases, and consequently it is not suitable for giving inventive solutions. Inventive solutions can be reached but at a price of an additional voluntary effort made by the users. Creativity is not directly stimulated by this approach. Another limit appears when the system cannot retrieve a sufficiently similar case or worse there is not any proposed solution; for example when the memory does not contain sufficiently cases. Then the proposed solution can be inappropriated and the designer must reach a solution with another method.

CBR is an interesting method in a relatively restricted domain, where the initial problem has its evolutions. Consequently solutions are locked up in a specific field of knowledge which is called psychological inertia. Indeed psychological inertia traduces our natural tendency to be convinced that the solution of our problem is in our competences field. This concept can be defined as a voluntary restraint for solution research. This can be very:

- Useful for routine design because most of the time, the solution is in your engineering field and you can reach it rapidly.
- Penalizing for rupture design, because you have to enlarge your knowledge (outside your engineering field) in order to propose inventive solutions.

CBR is based on the similarity between two problems: one to solve and the other one yet solved. When there is a tiny difference between both of them, it is supposed that the solution of the solved problem can be applied to the problem solved. Considering the typology proposed by Gero [17], most of the CBR systems dedicated to design correspond to routine design. Indeed in CBR, it is considered that a new design is near a past one, consequently creativity is not directly stimulated. While CBR application for repetitive design is obvious, its use for inventive design (creation of new knowledge for a company, a group) is more limited. In inventive design, problems are totally new and the required solutions are very distant from those already known.

Some drawbacks of the CBR approach like the problems of the psychological inertia, low level of innovation, absence of prediction, or no retrieved case, can be avoided by a method which changes the level of abstraction of the problem resolution; the TRIZ theory. It allows the passage from routine design to inventive design.

3. TRIZ

3.1. General presentation

Concerning inventive problem solving, there is a strong belief that this is a psychologically driven activity. For many people, innovation arises from higher intellect, chance or a process out of human control. But in order to stimulate innovative ideas some methods were created: trial and errors, brainstorming, etc. With these methods, designers try to access (reach) to their whole knowledge instead of increasing it. The main advantage of these methods is that they are easy to understand and to implement. But their principal drawback is that they explore in a random way the solution space. Consequently, the time and the cost to generate a solution are very important. Moreover, the solution found is often a trade-off with a low level of innovation (in the way of Table 1). However, a theory that refuses trade-off has appeared: TRIZ (Russian acronym for "Theory of Inventive Problem Solving"). This theory comes from with the idea that every engineer can; become an inventor, solve very difficult problems, and propose innovative solutions. TRIZ is an inventive problem solving method that increases the ability to solve creative problems. TRIZ has its origins in the former USSR, where it was founded by Altshuller [3].

One of the main advantages of TRIZ is that the solution space is not explored randomly. Accounting for problem constraints, the resolution tools of TRIZ give directions to explore in order to find a solution. Consequently, TRIZ has the capacity to considerably restrict the research space for innovative solutions, guide thinking towards solutions or strategies that have demonstrated their efficiency in a past similar situation, and produce an environment where the generation of a potential solution is almost systematic [18].

Of course TRIZ does not give directly an applicable solution but it proposes research directions to find solutions, then it leaves place to the designer creativity. With TRIZ, people are able to generate better ideas faster (because they are placed in a favourable environment) and have a basis for selecting the best ideas. TRIZ is not an ideal theory, it has several drawbacks. Even if it is more and more used in companies (in every technical domain), TRIZ is complex to understand, but nowadays efforts are made to simplify it [19].

The most important source of TRIZ has been patents and technical informations. But this theory is also based on:

- Analysis of million of patents and tools coming from them.
- Analysis of scientific literature (list of effects extracted from various scientific fields).
- Analysis of psychological behaviour of inventor.
- Analysis of existing methods and tools.

The main result of these analysis is the collection of TRIZ concepts and tools that helps to solve non-routine problems. These concepts and tools give access to the best practices in the whole technical domain thus increasing the creative potential of designer.

As Domb [20] explains, the three primary findings of this research are as follows:

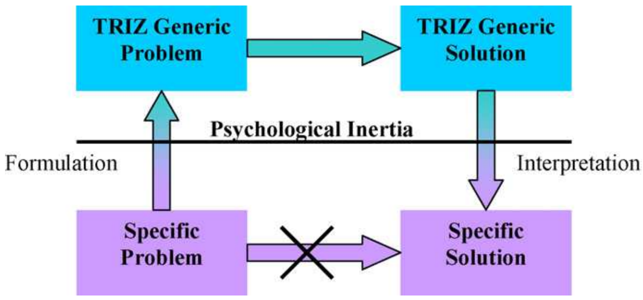

Fig. 2. TRIZ problem solving reasoning.

(1) Problems and solutions were repeated across industries and sciences.
(2) Patterns of technical evolution were repeated across industries and sciences.
(3) Innovations used scientific effects outside the field where they were developed.

This huge work establishes a knowledge base which is used in the tools and heuristics of TRIZ. Each time a new problem is solved, the knowledge base becomes richer. As CBR, the basic assumption of TRIZ is analogy; it takes benefit of the similarity between the current problem and past ones. Nevertheless, the two main differences between TRIZ and CBR are:

- TRIZ is not specific to one technical domain but by its foundations it concerns all technological domains.
- TRIZ is based on technological evolutions and developments.

With TRIZ, the problem is elevated to a higher level of abstraction before being solved. Fig. 2 represents the general TRIZ problem solving process. During the patents analysis (from various engineering fields), with this level of abstraction, Altshuller discovered that very different technical systems and processes share similar peculiarities in their evolutions. For example the same generic problem had been pointed out and solved with the same generic principle of resolution but in different technical domains and sometimes the solutions were separated by many years. With this level of abstraction, Table 1 (one conclusion of the patents analysis) expressed that inventions classified in levels 1–3 are usually transferable from one technical domain to another. This remark means that 95% of inventive problems in any domain have already been addressed and solved in some other fields. Hence, an inventive solution has a lot of chance to be useful in another domain. Consequently, Altshuller thought that if inventors can benefit from successful solutions found in others disciplines (and can access to those), the innovation process will be more efficient.

Finally, TRIZ theory encompasses a set of fundamental concepts, some tools and heuristics to solve complex problems. Among main TRIZ concepts and heuristics there are:

- *Laws of system evolution*. During its life cycle, a system is always evolving and this evolution is governed by objective laws. With this concept, it is possible to anticipate future ways of evolution of your system. There are 8 very generic laws (they are not rigorous mathematical laws as in physics, so they are usually referred as patterns).
- *Ideality*. Ideality is a goal. All systems evolve towards the increase of their degree of ideality. One way to measure the ideality is to use the Ideal Final Result (IFR). It is a psychological concept that allows to find the best solution for a complex problem without taking into account cost, time, space or any problem constraints. It defines a sort of "virtual" goal. This ideal system is often a utopian system but it guides reflexion toward seldom-explored direction.
- *Contradiction*. In TRIZ, problems can be written in terms of contradiction. An inventive problem contains at least one contradiction, and an inventive solution overcomes totally or partially this contradiction. A contradiction is a conflict in the system. Contrary to classical method for creativity stimulation (brainstorming, trial and errors, etc.), TRIZ refuses trade-off and tries to eradicate the contradiction. A clearly defined problem equals the formulation of its main contradiction and stands near solution. A contradiction arises when two requirements or needs for a system are mutually exclusive but both must be associated to reach the system objective. Several types of contradictions have been identified, but in this article only physical and technical ones are defined. Technical contradictions exist when any tentative to improve the performance of a useful function of a system, produces as a consequence an unacceptable deterioration in a second useful function in the system. It represents a conflict between two subsystems. A physical contradiction occurs when a component or element in a system present two mutually exclusive states simultaneously: a surface must be smooth and rough. It represents a conflict in the same subsystem. TRIZ has specific tools to solve these contradictions.

All TRIZ concepts implemented in various tools can be divided in 3 categories: tools to model problem (Innovation Situation Questionnaire (ISQ), Problem Formulation, Substance-Field Analysis, etc.), tools to break psychological inertia during formulation and interpretation steps (Fig. 2) (Ideal Final Result, Nine Screens, Dimension Time Cost operators, Miniature Dwarfs, etc.), tools to solve generic problems (Scientific Effects, Principle Separation, Contradiction Matrix and 76 standard solutions). The contradiction matrix is the key milestone of our model, consequently only this tool is presented and detailed in the following part.

3.2. *Contradiction matrix*

Altshuller and his research team collected examples of repeated use of the same solutions from patents informations. After its patents analysis, Altshuller has concluded that technical innovation comes from a limited number of research directions for solutions (how people solved problems) for all technical domains; he called them principles. After a painstaking work, the good solutions were sum up into 40 principles. Of course, principles do not give the solution but they limit the solution domain for research, giving ways to reach a solution (in Fig. 2 principles are TRIZ generic solutions). The interpretation of principles to find a solution is the expression of the user creativity. These principles are detailed in sub-principles in order to increase their efficiency. For example, we give some possible interpretations of the Principle 26 entitled *Copying*, which is decomposed into two sub-principles:

(A) *Instead of an unavailable, expensive, fragile object, use simpler and inexpensive copies.*

Use of virtual reality in process instead of real tests: in operator formation, changing of operating conditions for example.

(B) *Replace an object or process with optical copies.*

Use of pictures and image treatment to measure particles dimension (to determine particle distribution) or to measure flow characteristics PIV technique...

Damaged Parameter

Improved Parameter	1	2	3	4	5	6	7	8	9	10
1			15, 8 19, 34		29, 17 38, 34		29, 2 40, 28		2, 8, 15, 38	8, 10, 18, 37
2				10, 1, 29, 35		35, 30, 13, 2		5, 35, 14, 2		8, 10, 19, 35
3	8, 15, 29, 34				15, 17, 4		7, 17, 4, 35		13, 4, 8	17, 10, 4
4		35, 28, 40, 29				17, 7, 10, 40		35, 8, 2,14		28, 10
5	2, 17, 29, 4		14, 15, 18, 4				7, 14, 17, 4		29, 30, 4, 34	19, 30, 35, 2
6		30, 2, 14, 18		26, 7, 9, 39						1, 18, 35, 36
7	2, 26, 29, 40		1, 7, 4, 35		1, 7, 4, 17				29, 4, 38, 34	15, 35, 36, 37
8		35, 10, 19, 14	19, 14	35, 8, 2, 14						2, 18, 37
9	2, 28, 13, 38		13, 14, 8		29, 30, 34		7, 29, 34			13, 28, 15, 19
10	8, 1, 37, 18	18, 13, 1, 28	17, 19, 9, 36	28, 10	19, 10, 15	1, 18, 36, 37	15, 9, 12, 37	2, 36, 18, 37	13, 28, 15, 12	

Principles to use

Fig. 3. Section of the contradiction matrix.

Refs. [21,22] propose chemical engineering examples for each of the 40 principles (and sub principles) in order to understand their meaning.

Moreover during the patents analysis, Altshuller notes that technical contradictions can be expressed in terms of conflict between two parameters: one improved and the other one damaged (TRIZ generic problem in Fig. 2). Only 39 parameters were extracted to describe all the contradictions encountered in patents. Representing technical contradiction as a combination of two parameters requires a broad interpretation of them, so they are generic for many engineering fields.

Parameters and principles are put together in a tool where we have the contradiction formulation (problem formulation) and ways to solve it (principles). Finally, they built a 39×39 matrix. On the line, is located the improved parameter, on the column the damaged one. For one contradiction, the cell at the intersection of the line and the column indicates the principle(s) to explore in order to solve it (Fig. 3). Through the contradiction matrix, TRIZ opens up the world patents bases for identifying principles that may offer possible solutions.

To eliminate a technical contradiction a five steps method is used:

Step 1: Traduce the problem in the contradiction between two parameters.
Step 2: Identify both parameters among the 39.
Step 3: Use the matrix.
Step 4: Identify the principle to use. In the intersection cell the principles are classified in a statistic recommended order of use for contradiction resolution.
Step 5: Traduce the principle in an operational solution (expression of the creativity).

During Step 4, if the principles proposed in the cell of the contradiction matrix do not generate a solution, the user can try to use the other ones.

An example of use of the contradiction matrix concerns deposit by chemical reaction during electronic components fabrication. Chemical vapour deposition (CVD) consists in putting in contact substrates with one or several reactive gas. Gas chemically reacts in order to deposit a solid film on substrates. One way to produce micro electronic components is to use a low-pressure chemical vapour deposition reactor (LPCVD) with a vertical configuration (Fig. 4a). While analyzing its performance, several drawbacks appeared but one, related to the reactor performance and configuration, seems to be more important. A contradiction is identified to improve the quality of the siliceous film in the wafer; the gap between wafers must be large. In consequence, the quantity of wafers inside the reactor is reduced affecting productivity (Step 1). The problem is stated as "To increase the productivity in the reactor without radically modifying its shape". The two parameters to state the generic problem are: "Productivity" to be improved but it degrades the "Shape" of our system (Step 2). In Step 3, the use of the contradiction matrix gives four inventive principles in the following hierarchical order: 14 (spheroidality), 10 (prior action), 34

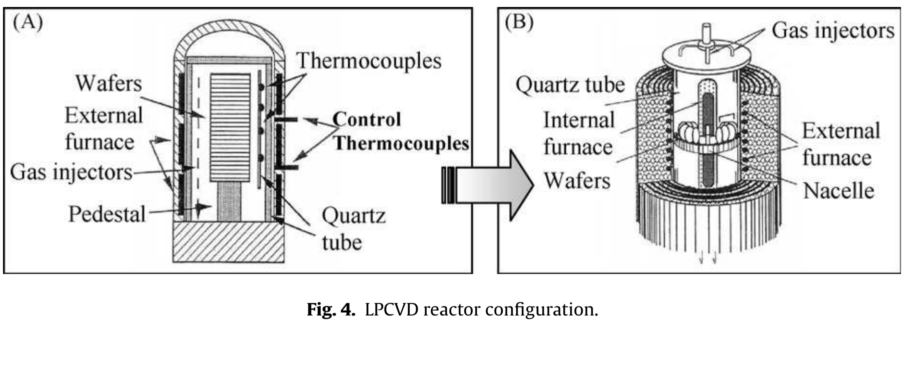

Fig. 4. LPCVD reactor configuration.

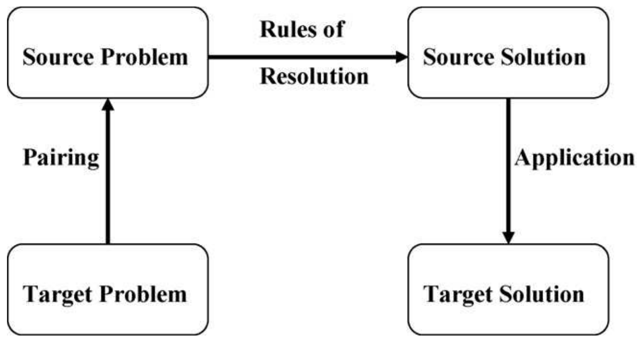

Fig. 5. CBR reasoning [27].

(rejecting and regeneration parts) and 40 (composite materials). In Step 4, we chose Principle 14 "spheroidality" that is decomposed into 3 sub principles:

- Replace linear parts or flat surfaces with curved ones, and cubical shapes with spherical shapes.
- Use rollers, balls, spirals domes.
- Replace linear motion with a rotating motion; utilize a centrifugal force.

One interpretation (Step 5) of this principle is to change the shape of the useful working area; it should be spherical. This solution is shown in Fig. 4b [23]. The new reactor has a 90 wafers capacity while the initial one has a 25 wafers capacity; consequently, the productivity is radically improved.

3.3. Comments on TRIZ

The first version of the contradiction matrix was an efficient tool to solve technical contradictions but it has been built in the 1950s and evolved until 1980s. With the evolutions of technical systems, this version becomes less efficient. Mann [24] has tested the matrix with new patents and found the patented solution for only 50% of them. Consequently, he has analysed many others patents and proposed another version of the matrix [25]. In this new version the number of parameters has been increased to 48 but the number of principles does not evolve (always 40). Moreover all the cells of the matrix were filled (except the diagonal cells because they correspond to physical contradictions: a parameter is improved and damaged simultaneously) which was not the case in the preceding version. This new version was tested and demonstrated its efficiency [26]. This is this new version that it is used in the synergy, part 4.

It is interesting to compare the way of reasoning in TRIZ and in CBR like in Estevez et al. [27]. They have schematized the CBR reasoning (Fig. 5). By comparison between Figs. 2 and 5, they clearly demonstrate the main difference between TRIZ and CBR: the level of abstraction for the reasoning purpose. In CBR, the level of abstraction is the same for the target and source problems and solutions, while in TRIZ the pairing between problems is realised at the generic level (change in the abstraction level). This difference explains the use of CBR for routine design and the use of TRIZ for inventive design.

TRIZ has numerous advantages but in the context of this article, three of them can be put in highlight: its capacity to stimulate creativity for everyone, the fact that it eliminates barrier between industrial domains (higher level of abstraction), and its reduced time to produce an inventive solution. Nevertheless, as it is said in the general presentation, TRIZ is a complex theory, this is why it has some difficulties for being established and used. For that reason, the synergy proposed is based on the contradiction matrix which is one of the easiest tools to understand and to use. Another drawback appears; each time you have a new problem, you have to redeploy the whole process of resolution which can be time consuming. The proposed synergy eliminates this drawback by coupling TRIZ with CBR. The synergy exploits the main advantages of TRIZ and CBR, in order to propose a model to accelerate the preliminary design phase in Chemical Engineering and to generate rapidly inventive ideas.

TRIZ appears after the opening of the former USSR. Now it is widely used in various domains and companies: aeronautic, car industry, electronics, etc. But till now, few researchers used TRIZ in Chemical Engineering for example; Braunschweig and Irons [28] for computer-aided tool, Busov et al. [29] for heat exchanger, Li et al. [30,31] for distillation systems, reaction–distillation systems, Hipple [32] for analysis failures, and Srinivasan and Kraslawski [1] for safer chemical processes, etc.

4. The synergy TRIZ–CBR

4.1. The coupling

First, the synergy is possible because both methods presented above are based on analogical reasoning. Some complementary characteristics between CBR and TRIZ are summarized in Table 2.

In one hand, TRIZ offers its ability to eliminate barriers between technical domain and consequently to propose inventive solutions, coupled with its capacity to give a way of solution whatever the problem faced. On the other hand, CBR brings a way to simply model knowledge and a memory to store cases, and the whole 5′R process to accelerate the resolution. Moreover, its specificity in a domain can be useful in the adaptation phase.

In this synergy the memory is crucial like in CBR in general. For simplicity of use and research efficiency during the retrieval step, the contradiction matrix is used to build the case base (memory), avoiding the creation of a specific tool. Further more, it is used for the case base indexation; therefore there is no need for a decision tree index.

Table 2
Comparison between CBR and TRIZ

CBR	TRIZ
Limited in a specific domain, barrier to the creativity	Extended to all technical fields, environment to stimulate creativity
Routine design	Inventive design
No solution if the initial problem has no sufficiently similar case	Gives a way of solution for each problem
Produces a solution from an initial guess	Produces a solution starting from "nothing"
Contains a memory: solutions produced rapidly, increases its efficiency by learning	No memory; resolution process redeployed each time
Easy for use, thanks to its affinity with human resolution process	Difficult to use because of its particular way to tackle problems, and the amount of tools

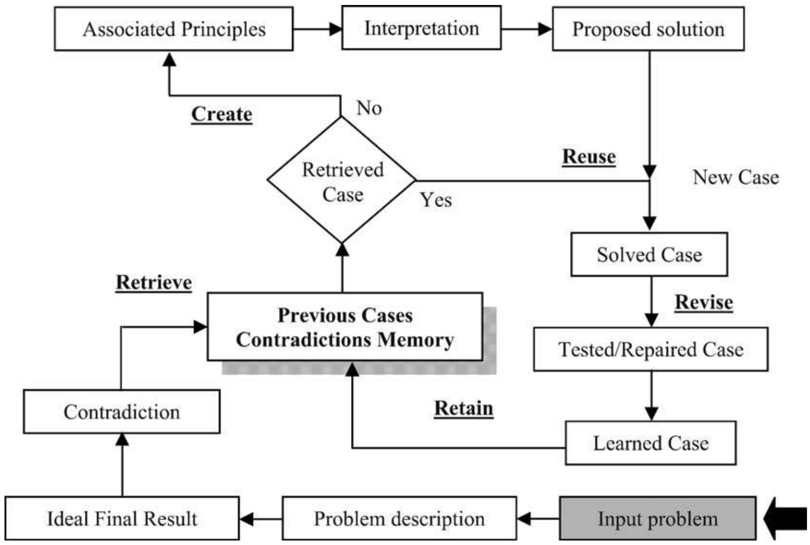

Fig. 6. TRIZ–CBR model.

Like in CBR, the central notion of the synergy is a case. The general definition of a case (1) is adapted here, for taking into account the specificity of the future use of the contradiction matrix. The use of the contradiction matrix as a memory imposes a way to structure cases. The problem is formulated with a contradiction and consequently with two parameters: the improved and the damaged ones. Of course, the two parameters are included in the relevant features for problem description but these only two parameters cannot describe precisely a problem and to ensure an effective retrieval. Consequently, others features are added in order to discriminate effectively cases:

- The system where the problem is located: reactor, distillation column, etc.
- The type of objectives: improvement of a characteristic, new functionality, eradication of a drawback, etc.
- The goal to reach: after a patents analysis, we notice that this feature can be expressed with one of the 48 parameters.
- The resources identified in the system: physical, chemical, liquid, solid, gas, etc.

With these five features, we can easily describe and discriminate cases. Concerning the two other components of a case, i.e. the solution and the comments, they stay as explained before in part 2 (in fact there are specific windows in which they are described), excepted for the solution in which one feature is added: the principle used to find it.

4.2. The model of the synergy

The model is presented in Fig. 6. Obviously, the preliminary step is to collect data on the handling problem and to describe it. Before filling the five features concerning the problem description, the ideal solution is also stated in order to propose a guide for the search direction of the future solution. Then the problem is stated as a contradiction coupled with the whole problem description (contradiction and the other features) used to explore the memory content for a similar problem. At this point of the synergy process, two different sub processes can take place:

(1) The retrieval offers a sufficiently similar problem or set of problems. Such a situation leads to the evaluation of the associated solutions to decide which solution or solving strategy has to be used as initial solution. Here the similarity between two problems is calculated with a similarity global function like Eq. (2).
(2) The memory does not have any similar solved case or sufficiently similar case (the similarity global function has a too small value). Under this condition, the system offers inventive principles associated to the contradiction, by which a satisfactory solution could be derived. The matrix finds its initial use.

Whatever the chosen sub-process, both converge to a proposed initial solution. Then this obtained solution is revised, tested and repaired if necessary with the aim to produce a satisfactory solution. Finally, this new solution is incorporated in the memory in order to be reutilized in the future. This learning step is very important because it allows to increase the cover of the problem space. It is important to underline that with this model we are sure to have an initial solution or ways to explore; it does not matter if the problem has a similar case or not. Moreover, during the resolution step, more than one solution could be found. In this situation, the ideal final result can be used as a criterion to rank them. But other criteria can be used like cost, etc.

The efficiency of this model, and more precisely of the tool built on it, is related to the number of cases stored in the memory. As we have underlined before, the second version of the contradiction matrix contains 48 parameters, consequently it can formulate 2256 contradictions (the diagonal is excepted because it is composed of physical contradictions). To ensure a good proposal for the initial solution, the memory needs to be filled with a large number of cases. Currently, we analyse more than 100 patents, we identify the contradiction, find the principle applied for the solution and finally describe the problem and its solution with the case formulation presented before. This work is still under development, nevertheless the tool based on this model is used and the learning step will accelerate the increasing efficiency of the memory.

As we just mentioned, a specific tool, based on this model, is created because CBR or TRIZ existing tools are not appropriate for the implantation of the TRIZ–CBR synergy; they are too much specific.

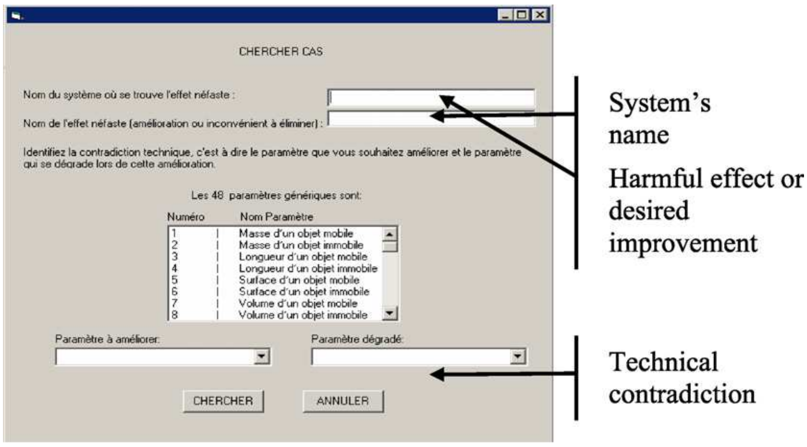

Fig. 7. The minimal requisites for search in the memory.

Even if the problem description contains five features, the minimal search engine utilizes three elements: contradictions, system, and harmful effect or desired improvement as represented in Fig. 7.

Estevez et al. [27] propose another way to combine CBR and TRIZ for inventive design. In their approach, CBR will be used for inventive design. To extend CBR from routine to inventive design, they exploit TRIZ problem solving reasoning (Fig. 2), with the aim of applying the pairing of generic resolution rules (increasing the level of abstraction of the CBR method). This work is still under development.

4.3. *Advantages–drawbacks*

This synergy allows to accelerate the resolution of problems by the use of past experiences in the domain of application but also in other domains by the way of TRIZ. The transdisciplinarity between domains allows to access to the best solutions, methods and practices in all technical domains which lead in more inventive solutions. With this synergy, the user is not unclosed in its domain but is more open-minded and breaks its psychological inertia.

The capacity of the synergy to give a research direction for the solution is another positive point. While there is a similar case in the memory or not, the system can offer a solution or a way to explore in order to find a solution. This is a great advantage compared to the CBR alone. Moreover with the memory, the knowledge is capitalized, stored and can be accessible and used by anyone. This gives to the tool a collaborative aspect.

Nevertheless, this approach has several limits. The first one is related to the difficulty to understand and to use TRIZ tools as we have mentioned before. But in this synergy, we avoid a great part of this limitation by using the easiest TRIZ tool and concept. The filling of the memory is probably the main limit of the synergy. As we explained before, many cases have to be stored in order to widely cover the problem space and to ensure the effectiveness of the tool. Of course the learning step is a way to overcome this difficulty and to benefit of all the potentialities of the memory in the future. Another limit is in the problem formulation and more precisely in the contradiction formulation. Very complex problems often have more than one contradiction. The difficulty is to find the main contradiction; the contradiction that once eliminated, the others or several other ones are withdrawn. During the problem elaboration, some TRIZ tools could be added in order to help to determine the contradiction: Innovative Situation Questionnaire, Problem Formulator or Root Contradiction analysis.

5. Example

The goal of this part is to demonstrate how the tool works and to present its functionalities on a mere example of Chemical Engineering. As we are going to see, even if it is simple, this example puts in highlight a limit of the model.

SMB is a chromatography technique to continuously separate multiple components mixture. This old technique has recently received a new researcher interest [33,34] because of its application in new areas such as biotechnology, pharmaceutical, fine chemistry, etc.

In fact, the SMB technique is based on the True Moving Bed (TMB) one. The TMB has been improved to become the SMB. Starting with the TMB approach and applying the tool based on this synergy, we are going to exemplify the two sub-processes: in one part we find the SMB technique, and in the other part we propose a preliminary design to the problem.

In the TMB process (Fig. 8), liquid and solid flow in counter-current directions. The liquid flowing out of zone 4 is recycled in zone 1, while the solid is recycled from zone 1 to zone 4. The solution to separate is fed continuously in the middle of the system.

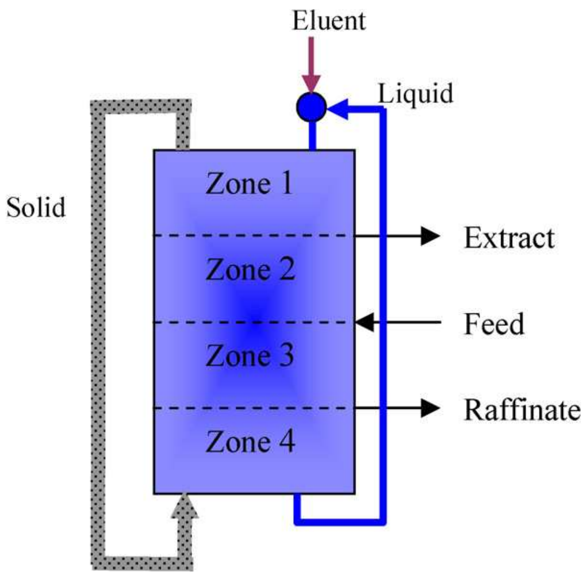

Fig. 8. True moving bed.

Another inlet allows to inject eluent. Two outlet product lines allow to withdraw products:

- Extract: rich in compound more retained (preferentially in the solid phase).
- Raffinate: rich in less retained compound (moving upward in the liquid phase).

The principal drawback of the TMB technique is the circulation of the solid phase, which is not an easy task.

The first step is to elaborate the case, information are collected for this. Following the process described in Fig. 6, the ideal final result is formulated: "Components of the mixture are separated by themselves, i.e. with no external means (no solid, etc.)". Of course it is a utopian solution but it is the final goal to reach. The solution proposed will be a stage in the direction of the ideal final result.

- To solve the TMB problem, the drawback has to be expressed in terms of contradiction. The ISQ is helpful to formalize this contradiction. With the ISQ, we have to answer to six principal questions, each one divided into sub-questions in order to set correctly the problem.

With the answers of the ISQ, the contradiction may be formulated: "reduce the circulation of the solid phase without decreasing the separation performance and increasing the operating cost". The next step is to identify the two parameters in the Altshuller's matrix:

- Improved parameter: convenience of use, parameter 33.
- Damaged parameter: energy spent by a moving object, parameter 19.

Now, the contradiction is established, it corresponds to only one feature of the problem description. Thus, before the retrieval step, the five features of the case must be filled:

- *Contradiction*: parameter 33 versus parameter 19.
- *System*: unit separation.
- *Type of goal*: eliminate a harmful effect.
- *Goal* (*indicated by a parameter*): function efficiency (parameter 24).
- *Resources*: solid, liquid, chemical components, etc.

The retrieve process is launched with the similarity function (2). Here two possibilities can take place and we are going to explore both of them.

5.1. No sufficiently similar case

If in the synergy sub process, the memory does not find similar case to this target problem. Of course, it is not currently the case because the case base is filled with numerous chemical engineering operations among which SMB. The interest here is to demonstrate how the tool can help the user to propose a solution if he does not know a technique (SMB here) or if the situation is not covered by the case base.

The crossing of line 33 and column 19 of the matrix gives the followings principles: 1 Segmentation, 13 Inverse, and 24 Intermediary. The first principle specifies that the object or process can be fragmented into independent parts. Consequently with the interpretation of this principle, the first idea is to divide the system into independent zones. One of the sub-principles of principle 13 is "Make movable parts fixed and fixed parts movable". Having in

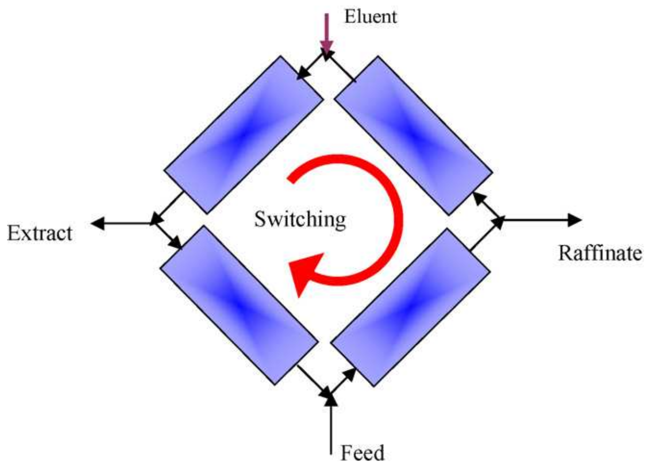

Fig. 9. Simulated moving bed.

mind that the circulation of the solid must be reduced, the solid can be fixed. Consequently if the solid becomes static, we have to perform the inlets and outlets ("fixed parts movable") in a rotating way in order to simulate fluid flows. Combination of both principles 1 and 13 gives the solution (SMB).

As it is clearly explained by Lim and Jorgensen [33], the counter-current flow of fluid and solid is simulated. The absorbent bed is divided into a number of fixed beds. The inlet and outlet lines move simultaneously to the next fixed bed, at fixed time intervals towards the liquid direction (Fig. 9).

5.2. Similar case

Here, we begin again at the retrieved step of the synergy but here the sub process one takes place. Of course with the same problem representation (starting from the TMB), the memory gives the SMB techniques as solution (because it is in the memory). However, the tool is not limited to give the principle of operation of the SMB but thanks to the problem input data, it gives a first design of the apparatus with some technical characteristics values: volumes, rotation frequency, etc. This first design can be used as a starting point for the solution to the initial problem. Then it must be corrected by simulation for example to correspond to the target problem.

Whatever the sub process, in the next step the proposed solution is revised. Once the problem solved, corrected and validated it can be stored in the memory.

5.3. Limit of the synergy

Always with the goal of increasing the function efficiency, the SMB can be improved. Here the elaborating stage is the same as before until the contradiction. A new contradiction is formulated and a new case is established with new features. For this second problem, the retrieved process finds a similar case, i.e. the sub process 2, and it gives a solution with a case in reactive distillation. This solution is adapted to our problem by using the SMB to make process intensification. A reactive part is incorporated to SMB in order to couple reaction and separation. The solid can be used as a catalyst for the reaction. In this evolution the SMB is now segmented in eight parts instead of four, and becomes the RSMB (reactive). Here the tool does not give a first design of the RSMB because this technique is not included in the memory yet. But, if we want to find directly the RSMB starting from the TMB, instead of SMB, we have to overcome two main contradictions: one from the TMB to the SMB, the other one from SMB to RSMB. But the synergy cannot treat simultaneously these two contradictions, we must consider them as two successive different cases. Consequently we cannot directly find the RSMB, without passing through an intermediary step. This is an important limit of our synergy because complex problems are often solved by overcoming several contradictions (simultaneous contradictions or successive contradictions). Nevertheless, the tool takes into account the possibility to connect successive contradictions for the same problem by making them dependent.

6. Conclusion and perspectives

This paper proposes a method to accelerate inventive design in Chemical Engineering. This method is based on the synergy between CBR and TRIZ. The presented model offers a way to transfer the solution from an identified analogous problem to a new target problem, reducing effort and time in solving inventive problems. This approach combines the TRIZ ability to propose creative solving strategies applicable across domains, and a framework that closely relates knowledge and action. In addition, one of the ways to drive the inventive process consists in reusing knowledge that has been acquired. Another important part of this model is learning, which is in fact inherent to a CBR system. For that reason, it is a good way to share knowledge. This model has been implemented in a computational tool. The possibilities of the synergy are demonstrated through a mere example but its potential strength is currently used on an industrial example.

Concerning the tool, it has to be improved by eliminating some limits presented before and by adding new functionalities. The adaptation step is crucial for the success of a proposed solution. For the moment the user does it himself but it can be helped in order to improve the whole process. A TRIZ tool, i.e. Substance-Field analysis, would be very useful because under certain conditions it gives more precise ways to solve problem. This tool is one stage for our main goal, which is to propose a tool to help the designer from the analysis of the problem requirements, until the detailed design, through inventive ideas generation and preliminary design. Here again, an automatic adaptation step will be very important in the detailed design.

Another future work is devoted to the fitting of TRIZ ontologies and tools to the specific cases encountered in the chemical process industry. Our idea in mind is to propose a methodology, and a tool to support innovation management in the field of Chemical Engineering for process design, operation, manufacturing and in future research areas such as micro processes, security aspects, and clean processes.

References

[1] R. Srinivasan, A. Kraslawski, Application of the TRIZ creativity enhancement approach to design of inherently safer chemical processes, Chem. Eng. Process. 45 (2006) 507–514.
[2] H.A. Simons, The Sciences of Artificial, Cambridge Press, 1969.
[3] G. Altshuller, Creativity as an Exact Science, Gordon & Breach, New York, 1984.
[4] R. Schank, Dynamic Memory: A Theory of Learning in Computers and People, Cambridge University Press, 1982.
[5] J. Kolodner, Case-based Reasoning, Morgan Kaufmann Publishers, Inc., 1993.
[6] Y. Avramenko, A. Kraslawski, Similarity concept for case-based design in process engineering, Comp. Chem. Eng. 30 (2006) 548–557.
[7] A. Kraslawski, I. Lyssov, T. Kudra, M. Borowiak, L. Nystrom, Case based reasoning for equipment selection using rough sets analysis in adaptation phase, Comp. Chem. Eng. (Suppl. 23) (1999) 707–710.
[8] T. Virkki-Hatakka, A. Kraslawski, T. Koiranen, L. Nystrom, Adaptation phase in case based reasoning system for process equipment selection, Comp. Chem. Eng. (Suppl. 21) (1997) S643–S648.
[9] I.R. Roda, M. Poch, M. Sanchez-Marre, U. Cortes, J. Lafuente, Consider a case-based system for control of complex processes, Chem. Eng. Prog. (1999) 39–45.
[10] J. Surma, B. Braunschweig, Case-base retrieval in process engineering: supporting design by reusing flowsheets, Eng. Appl. Artif. Intell. 9 (4) (1996) 385–391.
[11] E. Pajula, T. Seuranen, M. Hurme, Synthesis of separation processes by using case-based reasoning, Comp. Chem. Eng. 25 (2001) 775–782.
[12] T. Seuranen, M. Hurme, E. Pajula, Synthesis of separation processes by case-based reasoning, Comp. Chem. Eng. 29 (2005) 1473–1482.
[13] J.M.P. King, R. Banares Alcantara, Z.A. Manan, Minimising environmental impact using CBR: an azeotropic distillation case study, Environ. Model. Soft. 14 (1999) 359–366.
[14] Y. Avramenko, L. Nystrom, A. Kraslawski, Selection of internals for reactive distillation column—case based reasoning approach, Comp. Chem. Eng. 28 (2004) 37–44.
[15] Y. Avramenko, A. Kraslawski, Decision supporting system for pre-selection of column internals in reactive distillation, Chem. Eng. Process. 44 (2005) 609–616.
[16] I. Lopez-Arevalo, R. Banares-Alcantara, A. Aldea, A. Rodriguez-Martinez, L. Jimenez, Generation of process alternatives using abstract models and case based reasoning, Comp. Chem. Eng. 31 (2007) 902–918.
[17] J.S. Gero, Design prototypes: a knowledge representation schema for design, AI Magazine 11 (4) (1990) 26–36.
[18] J. Hipple, Solve problems inventively, Chem. Eng. Prog. 101 (4) (2005) 44–50.
[19] K. Rantanen, E. Domb, Simplified TRIZ: New Problem Solving Applications for Engineers and Manufacturing Professionals, St Lucie Press, Boca Raton, 2002.
[20] E. Domb, Managing creativity for project success, in: Proceedings of the 7th Project Leadership Conference, 2000.
[21] J. Hipple, 40 inventive principles with examples for chemical engineering, 2005 (http://www.triz-journal.com/archives/2005/06/index.htm).
[22] G. Cortes Robles, S. Negny, J.M. Le Lann, Another vision of the 40 inventive principles with applications in chemical engineering, 2005 (http://www.triz-journal.com/archives/2005/12/index.htm).
[23] H. Vergnes, Etudes expérimentales et modélisation du réacteur annulaire et de son modèle réduit, Ph.D. Thesis at the I.N.P. Toulouse, 1996.
[24] D. Mann, Assessing the accuracy of the contradiction matrix for recent mechanical inventions, 2002 (http://www.triz-journal.com/archives/2002/02/e/index.htm).
[25] D. Mann, S. Dewulf, B. Zlotin, A. Zusman, Matrix 2003, Updating the Contradiction Matrix, Creax Press, Belgium, 2003.
[26] D. Mann, Comparing the classical and new contradiction matrix. Part 2. Zooming in, 2004 (http://www.triz-journal.com/archives/2004/07/index.htm).
[27] I. Estevez, S. Dubois, N. Gartiser, J. Renaud, E. Caillaud, Le raisonnement à partir de cas est il utilisable pour l'aide à la conception inventive, in: Proceedings of 14 Atelier de Raisonnement à Partir de Cas Besançon, France, 2006, pp. 123–129.
[28] B. Braunschweig, K. Irons, TRIZ and evolution of CAPE tools from flowtran to cape-open and beyond, Eur. Symp. Computer Aided Process Eng. 12 (2002) 859–864.
[29] B. Busov, D. Mann, P. Jirman, Case studies in TRIZ: a novel heat exchanger (use of function analysis modeling to find and eliminate contradictions), 1999 (http://www.triz-journal.com/archives/1999/12/b/index.htm).
[30] X.N. Li, B.G. Rong, A. Kraslawski, TRIZ-based creative retrofitting of complex distillation processes—an industrial case study, Eur. Symp. Computer Aided Process Eng. 11 (2001) 439–444.
[31] X.N. Li, B.G. Rong, A. Kraslawski, Synthesis of reactor/separator networks by the conflict based analysis approach, Eur. Symp. Computer Aided Process Eng. 12 (2002) 241–246.
[32] J. Hipple, Use TRIZ in reverse to analyse failures, Chem. Eng. Prog. 101 (5) (2005) 48–51.
[33] Y.I. Lim, S.B. Jorgensen, A fast accurate numerical method for solving simulated moving bed (SMB) chromatographic separation problem, Chem. Eng. Sci. 59 (2004) 1931–1947.
[34] L.S. Pais, J.M. Loureiro, A.E. Rodrigues, Modeling strategies for enantiomers separation by SMB chromatography, AIChE J. 44 (3) (1998) 561–569.